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_____ WFEE _____
Fee Worksheet

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REV 7.02.03

10723208

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FILE 'HOME' ENTERED AT 13:17:19 ON 02 SEP 2004

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'CAPLUS' ENTERED AT 13:17:40 ON 02 SEP 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 2 Sep 2004 VOL 141 ISS 10
FILE LAST UPDATED: 1 Sep 2004 (20040901/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

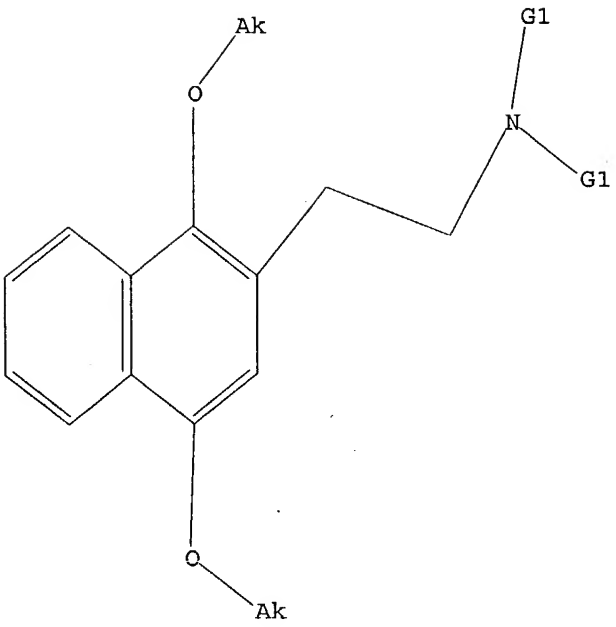
=>
Uploading 10723208.str

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR

Kamal Saeed

10723208



G1 H,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
REGISTRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 13:18:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 244 TO ITERATE

100.0% PROCESSED 244 ITERATIONS 19 ANSWERS
SEARCH TIME: 00.00.01

L2 19 SEA SSS FUL L1

L3 7 L2

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.44	156.95

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Kamal Saeed

10723208

FILE COVERS 1907 - 2 Sep 2004 VOL 141 ISS 10
FILE LAST UPDATED: 1 Sep 2004 (20040901/ED)

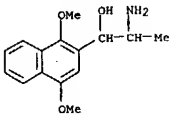
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 7 L2

=> d ibib abs hitstr tot

Kamal Saeed

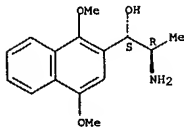
L4 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



● HCl

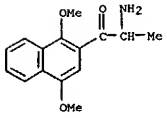
RN 477904-64-6 CAPLUS
CN 2-Naphthalenemethanol, .alpha.-[(1R)-1-aminoethyl]-1,4-dimethoxy-, hydrochloride, (.alpha.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

RN 477904-70-4 CAPLUS
CN 1-Propanone, 2-amino-1-(1,4-dimethoxy-2-naphthalenyl)-, hydrochloride (9CI) (CA INDEX NAME)

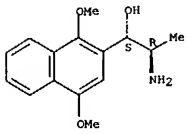


● HCl

L4 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 477904-73-7 CAPLUS
CN 2-Naphthalenemethanol, .alpha.-[(1R)-1-aminoethyl]-1,4-dimethoxy-, (.alpha.S)- (9CI) (CA INDEX NAME)

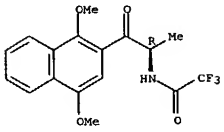
Absolute stereochemistry.



IT **477904-77-1P**, N-[(R)-2-(1,4-Dimethoxynaphthalen-2-yl)-1-methyl-2-oxoethyl]-2,2,2-trifluoroacetamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of novel naphthylaminopropane analogs with 5-HT2 receptor activity for use in the treatment of glaucoma)

RN 477904-77-1 CAPLUS
CN Acetamide, N-[(1R)-2-(1,4-dimethoxy-2-naphthalenyl)-1-methyl-2-oxoethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

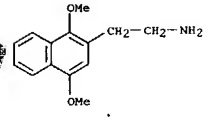
L4 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:561957 CAPLUS
DOCUMENT NUMBER: 129:297936
TITLE: The Frontier Orbital Phase Angles: Novel QSAR Descriptors for Benzene Derivatives, Applied to Phenylalkylamine Hallucinogens
AUTHOR(S): Clare, Brian W.
CORPORATE SOURCE: Division of Science, Murdoch University, Murdoch, 6150, Australia
SOURCE: Journal of Medicinal Chemistry (1998), 41(20), 3845-3856
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new empirical electronic descriptor, obtained from a MO calcn. and applicable to benzene derivs., is proposed. It is shown that this descriptor, the frontier orbital phase angle, correlates very strongly with the pharmacol. activity in humans of a large series of hallucinogenic phenethylamines. In the largest QSAR study on such hallucinogens yet reported, it is demonstrated that the phase of mixing of degenerate frontier orbitals of benzene to form the frontier orbitals of the drug results in the best electronic descriptor yet found for hallucinogenic activity in phenylalkylamines.

IT **207740-21-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(frontier orbital phase angles as QSAR descriptors for benzene derivs. applied to phenylalkylamine hallucinogens)

RN 207740-21-4 CAPLUS
CN 2-Naphthaleneethanamine, 1,4-dimethoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

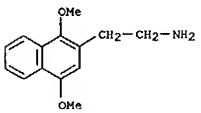
L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:207521 CAPLUS
DOCUMENT NUMBER: 129:12305
TITLE: Three-dimensional quantitative structure-activity relationships of hallucinogenic phenylalkanamine and tryptamine derivatives. Studies using comparative molecular field analysis (CoMFA)
AUTHOR(S): Beuerle, Gerald; Kovar, Karl Artur; Schulze-Alexandru, Meike
CORPORATE SOURCE: Inst. Pharmacy, Eberhard-Karls-Univ., Tuebingen, D-72076, Germany
SOURCE: Quantitative Structure-Activity Relationships (1997), 16(6), 447-458
CODEN: QSARDI; ISSN: 0931-8771
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

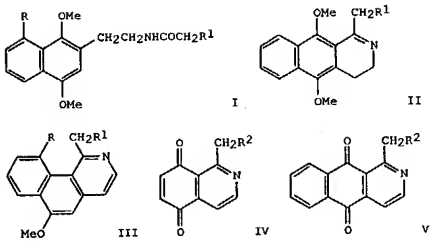
AB Investigations of the quant. structure - activity relationships of a data set comprising 66 phenylalkanamines have been carried out using the CoMFA method. This yielded a cross-validated correlation coeff. (q2 value) of more than 0.8. The target parameter used was the hallucinogenic effect on humans, since this variable is of particular importance for research into addictive substances. It was possible to confirm the reliability of the CoMFA anal. by using a second, independent phenylalkanamine data set. It was found that models with good predictive properties are obtained if up to ten components are taken into account. In a further step it was possible to include hallucinogenic tryptamine derivs. in a common Qsar anal. with the phenylalkanamines and this in spite of their differing basic structures. The final model from that the CoMFA plots were extd. is based on 148 compds. and permits precise inferences to be made concerning the relationships between structural elements and hallucinogenic effects.

IT **207740-21-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(QSAR of hallucinogenic phenylalkanamine and tryptamine derivs. using comparative mol. field anal.)

RN 207740-21-4 CAPLUS
CN 2-Naphthaleneethanamine, 1,4-dimethoxy- (9CI) (CA INDEX NAME)

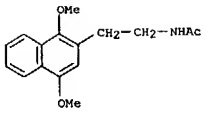


L4 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1988:549325 CAPLUS
DOCUMENT NUMBER: 109:149325
TITLE: Access to (aminomethyl)benzo[g]isoquinoline-5,10-diones. Abnormal substitution in the Bischler-Napieralski reaction of 1,4-dimethoxynaphthalenes
AUTHOR(S): Croisy-Delcey, Martine; Huel, Christiane; Bisagni, Emile
CORPORATE SOURCE: Lab. Synth. Org., Inst. Curie, Orsay, 91405, Fr.
SOURCE: Journal of Heterocyclic Chemistry (1988), 25(2), 661-5
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 109:149325
GI

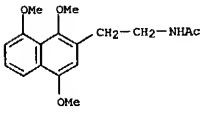


AB Bischler-Napieralski reaction of [(acylamino)ethyl]dimethoxynaphthalene derivs. I (R = H, R1 = H, phthalimido) gives the expected dihydrobenzoisoquinolines II (same R1). However, I (R = OMe, R1 = H, phthalimido) give only aromatized regioisomers III, and I (R = R1 = H) gives .apprx.30% III. Cyclocondensation of isoquinolinediones IV (R2 = H, NHAc, NHCOCOMe, NHCOCH2Cl) with AcO(CH:CH)2OAc gives 39-54% azaanthraquinones V (same R2).
IT **116577-58-3P 116577-59-4P 116577-63-0P 116577-64-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and Bischler-Napieralski reaction of, regiochem. of)
RN 116577-58-3 CAPLUS
CN Acetamide, N-[2-(1,4-dimethoxy-2-naphthalenyl)ethyl]- (9CI) (CA INDEX NAME)

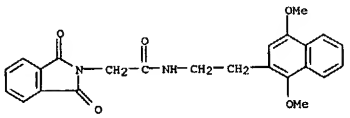
L4 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



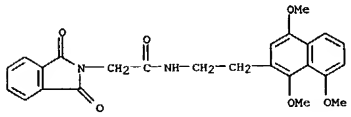
RN 116577-59-4 CAPLUS
CN Acetamide, N-[2-(1,4,8-trimethoxy-2-naphthalenyl)ethyl]- (9CI) (CA INDEX NAME)



RN 116577-63-0 CAPLUS
CN 2H-Isoindole-2-acetamide, N-[2-(1,4-dimethoxy-2-naphthalenyl)ethyl]-1,3-dihydro-1,3-dioxo- (9CI) (CA INDEX NAME)



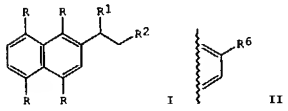
RN 116577-64-1 CAPLUS
CN 2H-Isoindole-2-acetamide, 1,3-dihydro-1,3-dioxo-N-[2-(1,4,8-trimethoxy-2-naphthalenyl)ethyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1985:523196 CAPLUS
DOCUMENT NUMBER: 103:123196
TITLE: 1,4,5,8-Tetraalkoxynaphthalene
PATENT ASSIGNEE(S): Otsuka Pharmaceutical Factory, Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

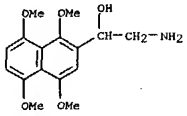
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 60100542	A2	19850604	JP 1983-209712	19831107
JP 04049536	B4	19920811		
PRIORITY APPLN. INFO.:			JP 1983-209712	19831107

OTHER SOURCE(S): CASREACT 103:123196
GI

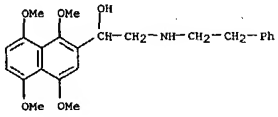


AB Title compds. I [R = alkoxy; R1, R2 = OH, alkanoyloxy, NR3R4; R3, R4 = H, alkyl, cycloalkyl, (un)substituted Ph, phenylalkyl] and their salts, useful as cardiovascular agents (no data), were prepd. Thus, treating 2.4 g II (R = OMe, R6 = CHO) with 1 g NaCN gave 2 g II [R = OMe, R6 = CH(OH)CN], 1.65 g of which was reduced in the presence of NaBH4 to give 500 mg II (R = OMe, R6 = CHOHCH2NH2), 310 mg of which was treated with 300 mg Me2CO in the presence of NaBH3CN to give 272 mg I (R = OMe, R1 = OH, R2 = NR3R4, R3 = H, R4 = CHMe2).
IT **98187-37-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reductive alkylation of)
RN 98187-37-2 CAPLUS
CN 2-Naphthalenemethanol, .alpha.-(aminomethyl)-1,4,5,8-tetramethoxy- (9CI) (CA INDEX NAME)

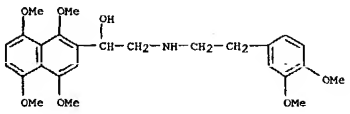
L4 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



IT **98186-93-7P 98186-96-0P 98186-99-3P**
98187-00-9P 98187-38-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 98186-93-7 CAPLUS
CN 2-Naphthalenemethanol, 1,4,5,8-tetramethoxy-.alpha.-[[(2-phenylethyl)amino]methyl]- (9CI) (CA INDEX NAME)

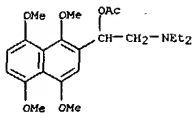


RN 98186-96-0 CAPLUS
CN 2-Naphthalenemethanol,
.alpha.-[[[2-(3,4-dimethoxyphenyl)ethyl]amino]methyl]-1,4,5,8-tetramethoxy- (9CI) (CA INDEX NAME)

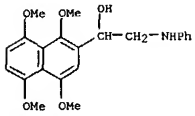


RN 98186-99-3 CAPLUS
CN 2-Naphthalenemethanol,
.alpha.-[(diethylamino)methyl]-1,4,5,8-tetramethoxy-, acetate (ester) (9CI) (CA INDEX NAME)

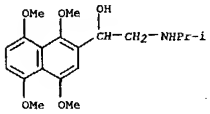
L4 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 98187-00-9 CAPLUS
CN 2-Naphthalenemethanol,
1,4,5,8-tetramethoxy-.alpha.-[(phenylamino)methyl]- (9CI) (CA INDEX NAME)



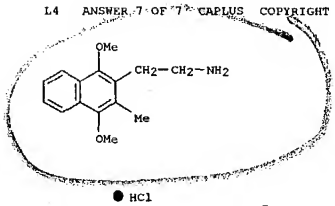
RN 98187-38-3 CAPLUS
CN 2-Naphthalenemethanol, 1,4,5,8-tetramethoxy-.alpha.-[[(1-methylethyl)amino]methyl]- (9CI) (CA INDEX NAME)



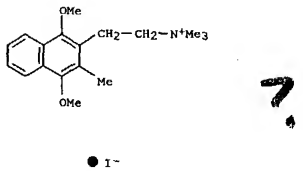
L4 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1969:47149 CAPLUS
DOCUMENT NUMBER: 70:47149
TITLE: Synthesis of 2-methyl-3-vinyl-1,4-naphthoquinones
AUTHOR(S): Bondinell, William E.; DiMari, Samuel J.; Frydman, Benjamin; Matsumoto, Kent; Rapoport, Henry
CORPORATE SOURCE: Univ. of California, Berkeley, CA, USA
SOURCE: Journal of Organic Chemistry (1968), 33(12), 4351-62
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Chlorobiumquinone (Ia), previously isolated from Chlorobium thiosulfatophilum and characterized as a 2-methyl-3-vinylmultiprenyl-1,4-naphthoquinone, is unique among natural multiprenylquinones in being a vinyl- rather than an allylquinone. Various approaches to the synthesis of 2-methyl-3-vinyl-1,4-naphthoquinone (I) derivs. were studied, and two general syntheses developed, both constructing the substituted vinyl side chain via the Wittig reaction. A primary requirement for both methods was a protecting protocol for the 1,4-O functions which would be inert to the ylide yet would allow generation of the quinone without destruction of the vinyl group. Such functionality was provided by the 1-pivalate ester-4-Me ether. These groups do not react with the ylide, and removal of the ester with LiAlH4 and oxidn. of the 1-hydroxy-4-methoxy compd. with FeCl3 gave quinone while leaving the vinyl side chain intact. One synthesis proceeded via 3-chloromethyl-4-methoxy-2-methyl-1-naphthyl pivalate which was converted into its tri-phenylphosphonium salt and thence to vinyl deriv. by generation of the naphthalenic ylide and reaction with a carbonyl component. The other synthesis utilized the 3-naphthaldehyde, prepd. from the chloromethyl compd. and K 2-propanenitronate, in reaction with the appropriate ylide. To avoid isomers, some secondary ylides were prepd. by alkylation of primary ylides. The relative advantages and disadvantages of both methods are considered. The separate, isomeric, vinyl compds. were obtained, and cis and trans stereochem. assignments made by relating their N.M.R. absorptions to those of unambiguous synthetic models. Various vinyl substitution patterns can be easily distinguished from the uv absorption of the resulting I derivs. 47 references.
IT **17827-38-2P 17827-57-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 17827-38-2 CAPLUS
CN 2-Naphthaleneethylamine, 1,4-dimethoxy-3-methyl-, hydrochloride (8CI) (CA INDEX NAME)

L4 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 17827-57-5 CAPLUS
CN Ammonium, [2-(1,4-dimethoxy-3-methyl-2-naphthyl)ethyl]trimethyl-, iodide (8CI) (CA INDEX NAME)



Kamal Saeed

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=> logoff
ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	34.64	191.59

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-4.90	-4.90

STN INTERNATIONAL LOGOFF AT 13:21:27 ON 02 SEP 2004

Kamal Saeed